



## **Efficient Modeling of Excitons in Type-II Nanowire Quantum Dots - Presented at: CLEO®/Europe-EQEC 2017, 2017, Munich**

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# Efficient Modeling of Excitons in Type-II Nanowire Quantum Dots

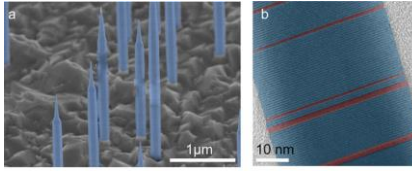
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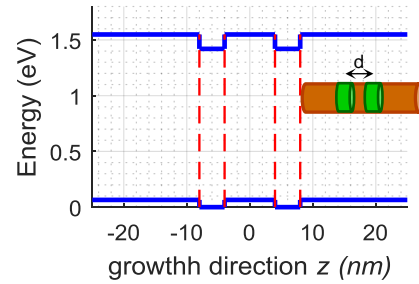
In nanowires, crystal phase quantum dots (QDs) can be synthesized by modifying the crystallographic structure as is shown in figure 1 [1]. This structuring can be made with atomic monolayer precision, and this good control of the geometry makes QDs in nanowires attractive systems for engineering quantum dot-based functionalities such as quantum gates. The crystallographic interfaces usually feature Type II band alignment, where electrons and holes are spatially separated onto the different polytypes, which is a key asset in implementing quantum gates. However, it also leads to very small oscillator strength (OS) in these structures compared to Type-I QDs.

In this work, we calculate exciton binding energy and oscillator strength using a full configuration interaction (CI) description of the few particle electron-hole system. Whereas widely used methods such as *ab initio* or tight binding are numerically demanding, the CI method is more efficient and thus suitable for engineering and design of quantum devices. We show that by engineering of a nanowire in double well QDs (DWQD) configuration, the oscillator strength, which is a key parameter in optical quantum gating in the STIRAP (stimulated Raman adiabatic passage) process for implementing quantum gates [2], is increased up to 10 times compare to single well QDs (SWQD). The initial ingredients of CI method for calculating the exciton state are the electron and hole single-particle wavefunctions and energies, which are obtained from the solutions of the three-dimensional Schrodinger equation within the envelope-function and effective-mass approximations. The few-particle Hamiltonian is then expanded within the bases of single-particle states. The exciton state is obtained by direct diagonalization of this Hamiltonian.

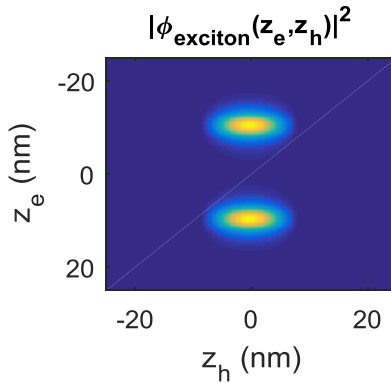
Figure 2 shows a nanowire DWQD bandstructure in the growth direction ( $z$ ) and its schematic in the inset. Figure 3 shows the calculated exciton wavefunction in the electron and hole coordinates in the  $z$  direction which shows the exciton is bounded in the barrier between quantum dots in the  $z_h$  coordinate. By changing the interdots distance, the normalized OS of the bound exciton can be increased up to 50%, as is shown in Figure 4, which is 10 times larger than what is calculated for ground state exciton in SWQDs.



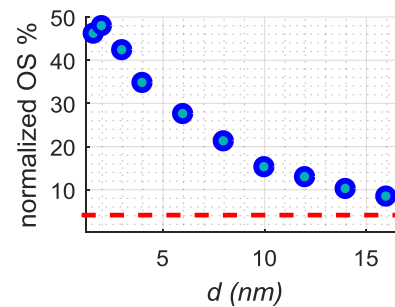
**Fig. 1** Scanning electron microscope image of the grown crystal phase InP nanowire QD.



**Fig. 2** InP nanowire DWQD band structure and its schematic in inset. Band structure parameters are from [1].



**Fig. 3** Bound exciton state in the  $z$  coordinate of electron and hole.



**Fig. 4** Normalize OS vs interdot distance  $d$  in nanowire DWQD. Dash red line shows normalized OS in nanowire SWQD.

## References

- [1] N. Akopian, G. Patriarche, L. Liu, J. C. Harmand, and V. Zwiller. "Crystal phase quantum dots." *Nano Lett.* **10**, 1198-1201 (2010).
- [2] T. Filippo, U. Hohenester, and E. Molinari. "High-finesse optical quantum gates for electron spins in artificial molecules," *Phys. Rev. Lett.* **90**, 206802 (2003)